A Coupling Method for Molecular and Continuum Models with Random Input Data Based on the Stochastic Collocation Approach

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In this work, we develop and analyze a stochastic method that couples atomic and continuum models with random parameters. The approach relies on two key ingredients: the Arlequin framework [1], which provides a convenient tool for concurrently coupling models of different natures, and the stochastic collocation technique [2, 3], which provides an attractive method for the treatment of random features by solving a set of deterministic problems. This new method is used to estimate the propagation of uncertainties for the determination of quantities of interest in multi-scale simulations. We present numerical experiments dealing with one-dimensional molecular chains and two-dimensional lattice structures to describe the technical features of this new stochastic method and demonstrate the performance of the proposed approach [4, 5].

References

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